NESDIS OPERATIONAL SOUNDINGS IN THE UPPER STRATOSPHERE

Tony Reale
NOAA/NESDIS/ORA
Forecast Products Development Team

1 INTRODUCTION

The following report addresses the National Environmental Satellite, Data, and Information Service (NESDIS) scientific procedures to retrieve the Advanced TIROS Operational Vertical Sounder (ATOVS) sounding products in the upper stratosphere. In summary, the procedures to derive operational soundings are separated into a series of Orbital processing and Offline processing steps (Reale et al. 2000); the later providing coefficients and data sets which are primarily based on collocated radiosonde and satellite observations. Such observations are compiled and updated on a daily basis (Tilley 2000), and directly accessed during Orbital processing as a source of first guess and retrieval solution information.

Since routine radiosonde observations are typically not available for the upper stratosphere, it is necessary to “artificially “extend the radiosondes above their respective, highest report level (to .1 mb) in order to provide some estimate of upper stratospheric first guess and solution data. The extension method was recently upgraded to utilize a statistical regression approach (Goldberg 1999) using available, collocated, Advanced Microwave Sounding Unit-A (AMSU-A) observations, with positive results.

The following paper outlines the current Online and Offline procedures to generate NESDIS sounding products in the upper stratospheric temperature.

2 ONLINE PROCESSING

Calibrated and limb-adjusted (Wark 1993) radiance temperature measurements for a given sounding location (Reale et al. 2000) are the basis for determining the first guess and derived soundings.

<u>The first guess</u> is computed using a library search technique (Goldberg 1988) which utilizes combinations of sounder measurements as discriminators for searching the respective “libraries” of collocated radiosonde and satellite observations. The libraries are segregated for clear and cloudy soundings, and terrain type (i.e., sea and nonsea).

The algebraic form for the library search is given in matrix equation 1:

$$D = (R - R_k)^t \; B^{-1} \; (R - R_k) \qquad (1)$$

where the subscript t indicates the matrix transpose, -1 the inverse, and

D : scalar closeness parameter,
B : sounding channel radiance covariance matrix; dimension (35 x 35),
R : adjusted, observed radiance temperature vector; channels FG (CC), and
R_k : adjusted, library radiance temperature vector; channels FG (CC).

The dimension "35" for the radiance covariance "B" matrix in Equation (1) denotes the total number of sounder channels, 15-channels for AMSU-A and 20-channels for the High resolution Infrared Radiation Sounder (HIRS) which comprise the complete suite of ATOVS measurements; not all are used. The "B" covariance matrices are computed using the satellite measurements stored on the first guess libraries (see Offline Processing). The channel combination FG(CC) are the specific channels used in the search to compute "D", and the subscript "k" is the number of library collocations searched, typically about 2000 per sounding. The specific channel combination, CC, and collocations searched,"k", depend upon whether the derived sounding is clear or cloudy, and over sea or non-sea terrain.

The first guess temperature, moisture and radiance temperature profiles for a given sounding are computed by averaging the 10 closest collocations; that is, those with the smallest D. Radiosonde averages are used for the guess temperature, and the limb-adjusted measurements from the sounder (including those not used in the search) are averaged for the guess measurement. **Beginning above 50 mb, where radiosonde observations become sparse, the report data (used to provide the first guess) are from extended radiosondes using a statistical regression of the collocated, AMSU-A, satellite measurements (see Offline).**

<u>The sounding retrieval</u> uses the Minimum-Variance-Simultaneous solution (Fleming et al. 1986) given by matrix equation (2):

$$T - T_g = S A^t \, (A S A^t + N)^{-1} \, (R - R_g) \qquad (2)$$

where the subscript t indicates the matrix transpose, -1 the inverse, and:

T: final soundings products vector, (133),
T_g: first guess products vector, (133)
S: first guess covariance matrix, (133 x 133),
A: sounder channel weighting matrix, (35 x 133),
N: measurement uncertainty matrix, (35 x 35),
R: observed radiance temperature vector, channels RE (CC), and
R_g : first guess radiance temperature vector, channels RE (CC).

The product vector (T) of length 133 includes 100 levels of atmospheric temperature (1000 mb to .1 mb), 32 levels of moisture (1000 mb to 200 mb), and a surface level. The dimension 35 for the A and N matrices denotes all the ATOVS channels; not all are used. The channels RE (CC) denotes the first guess and observed channels[1] used in the retrieval solution (2).

A total of thirty-two (32) unique combinations of S, A and N matrices, referred to as retrieval operators, are computed (see Offline) and available for the orbital retrieval step. The channel combination and retrieval operator used for a given sounding depends on the cloud and terrain designation.

3 OFFLINE PROCESSING

The two Offline processes which impact the computation of derived soundings are the compilation of **first guess libraries** and **retrieval coefficients**.

The first guess libraries consist of collocated radiosonde and satellite observations which are compiled and updated daily, and directly accessed during orbital processing. First guess libraries contain about 10,000 collocations of radiosonde and satellite observations, segregated by clear, cloudy, and terrain designations (Tilley et al. 2000). Candidate radiosonde observations require an initial vertical extent from at least 950 mb to 50 mb.

Figure 1 illustrates a typical global distribution of collocations stored on the first guess libraries for combined clear and cloudy soundings from NOAA-15. The sounding location is used for plotting, and the color coding for the collocated sounding is sea (light blue), land (dark green), coast (yellow), ice (grey) and snow (white). Collocations with ship radiosondes are red.

The compilation of first guess libraries includes an upward extension of each radiosonde temperature profile from the highest report level (i.e., at least 50 mb) to .1 mb, a critical step in the derivation of upper stratospheric sounding products. The original approach to do this was to simply use the collocated derived sounding and first guess information to extend each radiosonde. However, in April, 2000, a new approach to extend radiosondes using a statistical regression of the collocated AMSU-A measurements was deployed operationally. The regression coefficients are those provided by Goldberg (1999).

---

[1] Note that first guess observations for a given channel are available independent of whether it was used in the first guess search.

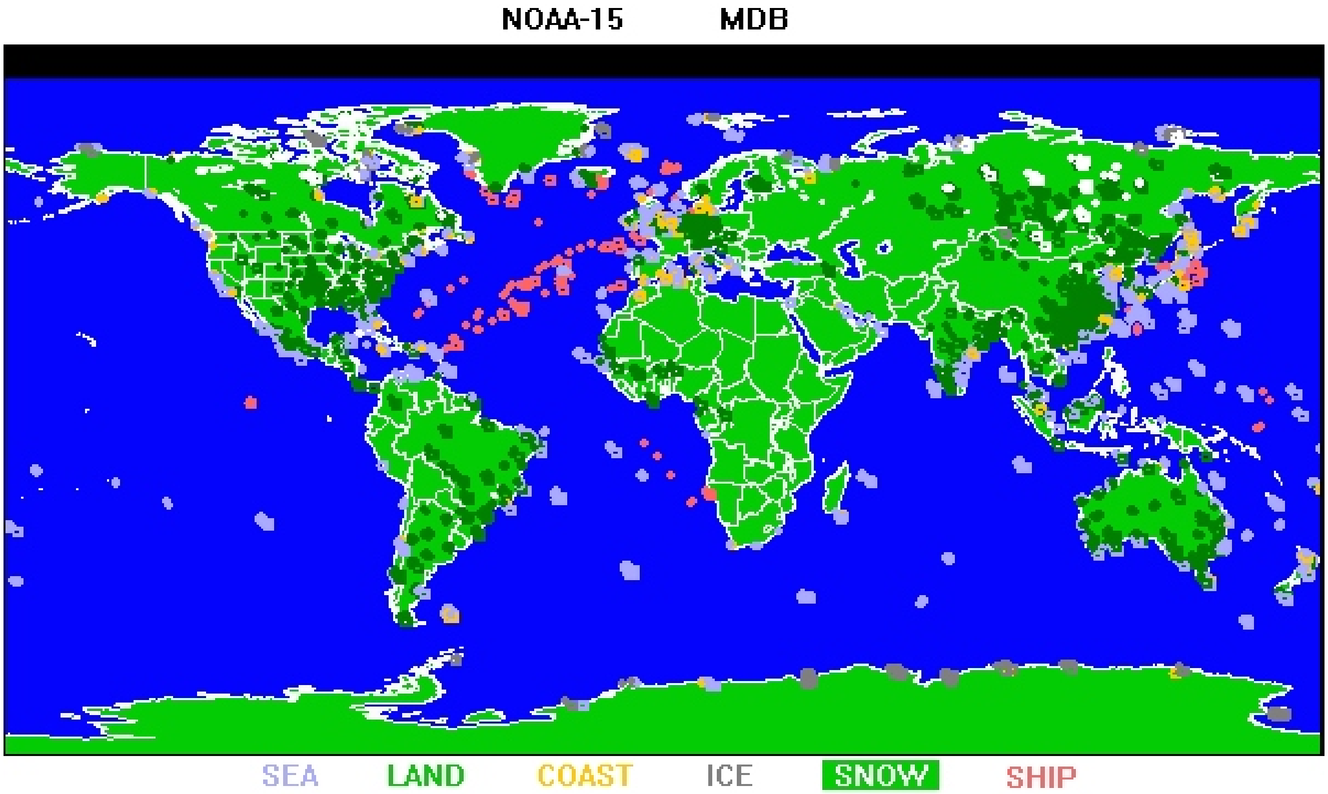

Figure 1: The global distribution of clear and cloudy collocations stored on the First Guess Libraries from NOAA-15 observed on September 6, 2000.

Requirements for extension include the comparison of regressed and observed radiosonde temperature profiles beginning at the highest report level[2] downward to 60 mb. A merge point is then defined as the level at which the two profiles differ the least. This minimum difference must be less than 2K absolute, otherwise the collocation is rejected, and is not stored in the library. Typically, less than 10% of the candidate collocations fail these criteria.

<u>The retrieval coefficients</u>, or retrieval operators, are updated weekly using the satellite and radiosonde collocations. As indicated in Equation 2, the retrieval operator consists of the:

- o A-matrix providing vertical weighting functions for each sounding channel,
- o the S-matrix providing the vertical covariance of first guess (or background) error, and
- o the N-matrix providing the sounder measurement uncertainty.

[2] No radiosonde data are retained at and above 10 mb.

Nine (9) "A" matrices (Fleming et al. 1986) provide the vertical weighting functions for each ATOVS sounding channel. Each matrix is computed based on combined samples of clear and cloudy collocations for selected latitude belts and terrain categories, respectively (Tilley 2000), and are the same for clear and cloudy soundings. Individual and mean profiles of the radiosonde report data, which include the "extended' upper stratospheric temperatures, and corresponding atmospheric transmittance profiles (McMillin 1995) are combined to compute an A-matrix for each collocation, which are then averaged to compute each of the nine A-Matrices available for retrieval. The A-matrix used for a given retrieval is consistent with the sounding latitude.

Four (4) "S" matrices (Fleming et al. 1986) provide the background error, defined as the vertical covariance of the "first guess minus radiosonde" differences for temperature (and moisture) at each level, including cross correlations between temperature, moisture and surface terms. Note that in the upper stratosphere, the first guess and radiosonde data are primarily based on regressed profiles from Goldberg (1999). Four (4) S-matrices are computed, consistent with the collocations searched to determine the first guess.

The "N" matrix is diagonal and contains the sounder measurement uncertainty values primarily determined from the calibrated sounder data.

A total of thirty-two (32) retrieval operators are available, each containing a unique combinations of the nine (9) A and N matrices, and the four (4) S-matrices as described above. Seven (7) operators are available for sea soundings, and nine (9) are available for nonsea soundings, respectively, with separate sets of operators for clear and cloudy sounding designations.

4 UPPER STRATOSPHERIC SOUNDINGS

Polar satellite data are a major source of global temperature information in the upper stratosphere (Finger et al. 1993). The following section provides data and results concerning upper stratospheric temperature sounding products provided by NESDIS.

The four panels of Figure 2 illustrate 12-hour, globally composited fields for AMSU-A channel 13 (upper left), which is sensitive in the vicinity of 5 mb, and corresponding 5 mb derived temperatures from ATOVS onboard NOAA-15 (upper right), and RTOVS onboard NOAA-14 (lower left). The NOAA-15 minus NOAA-14 temperature difference at 5 mb are shown in the lower right panel. The spectral, color scales are indicated below each panel, with identical scales used for the respective 5 mb temperature fields. Temperature difference scales range from +/- 15 K, with white indicating all differences between +/- 1.5 K.

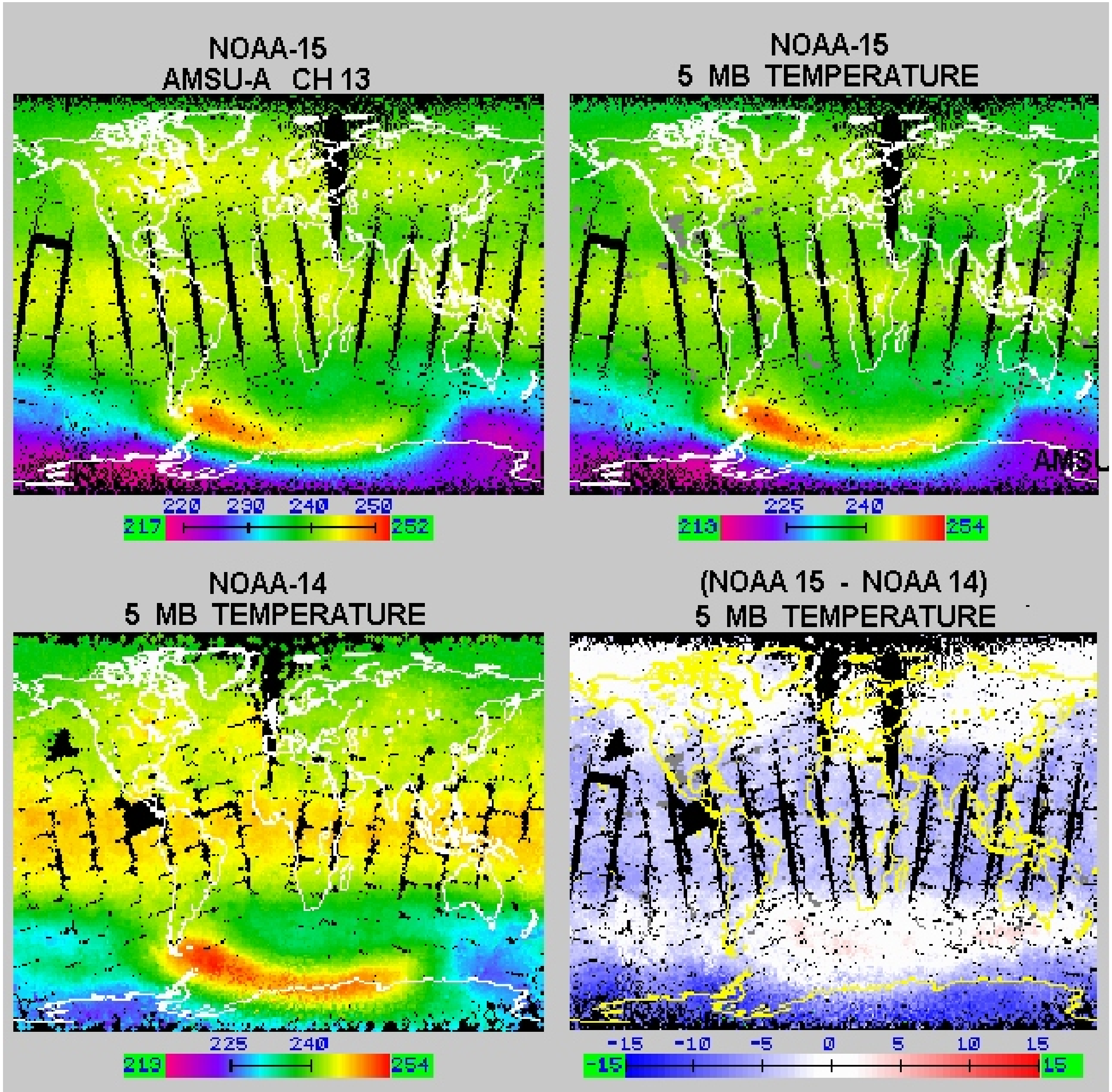

Figure 2: NOAA-15, AMSU-A channel 13 (upper left) and derived temperatures at 5mb (upper right), NOAA-14 derived temperatures at 5 mb (lower left), and NOAA-15 minus NOAA-14 difference field at 5 mb composite for the period 16Z to 05Z on September 6 and 7, 2000.

As seen in Figure 2, the 5 mb temperature patterns for the NOAA-15, ATOVS system, are tightly aligned with the channel 13 measurements, and differ significantly with their NOAA-14 counterparts. Absolute differences between these satellites are on the order of 5K over a large portion of the Tropics, and exceed 10K in south polar regions. Differences at other upper stratospheric levels (not shown) show similar magnitudes, including significant temperature lapse-rate differences between the ATOVS and RTOVS data.

The reason for these differences is primarily the new approach in ATOVS for extending the radiosondes stored in the first guess libraries using the statistical regression approach, as discussed earlier. Subsequent comparisons against available Halogen Occultation Experiment (HALOE) soundings above 10 mb have confirmed the improved performance of the ATOVS upper stratospheric products (Goldberg 1999).

The statistical regression coefficients used are actually a subset of those available to compute complete atmospheric soundings for climate applications. These coefficients are based on two separate samples of collocations, a fixed sample of collocated radiosonde and observed, NOAA-15, satellite measurements (Tilley et al. 2000) for pressure levels from the surface to 50 mb, and a historical sample of collocated radiosonde/rocketsonde (Finger et al. 1993) and calculated (McMillin 1995) satellite measurements for pressure levels above 50 mb to .1 mb. The latter are used to extend radiosondes.

Once extended, the radiosonde profile provides the first guess information (similar to lower levels) through the library search approach (equation 1), followed by the MVS retrieval (equation 2) to derive sounding products. Since the merge point for a given radiosonde can vary between 60 mb and 10 mb, the first guess information for a given sounding can result from a combination of radiosonde and regressed data at these levels, a potentially noise inducing process. This is constrained by the rejection of collocations for which the regressed and original radiosonde data exceeded 2 K.

An important question is how different are the NESDIS derived soundings from the original AMSU-only soundings from (Goldberg 1999) in the upper stratosphere. Figure 3 illustrates an example of differences at 5 mb for NOAA-15[3]. It can be seen that the differences at these levels are on the order of 2 degree K, significantly reduced from the original differences of five (5) to ten (10) K observed for RTOVS (N-14) versus ATOVS (N-15) in Figure 1.

[3] AMSU channel 14, the highest peaking channel at about 2 mb., is not available for N-15.

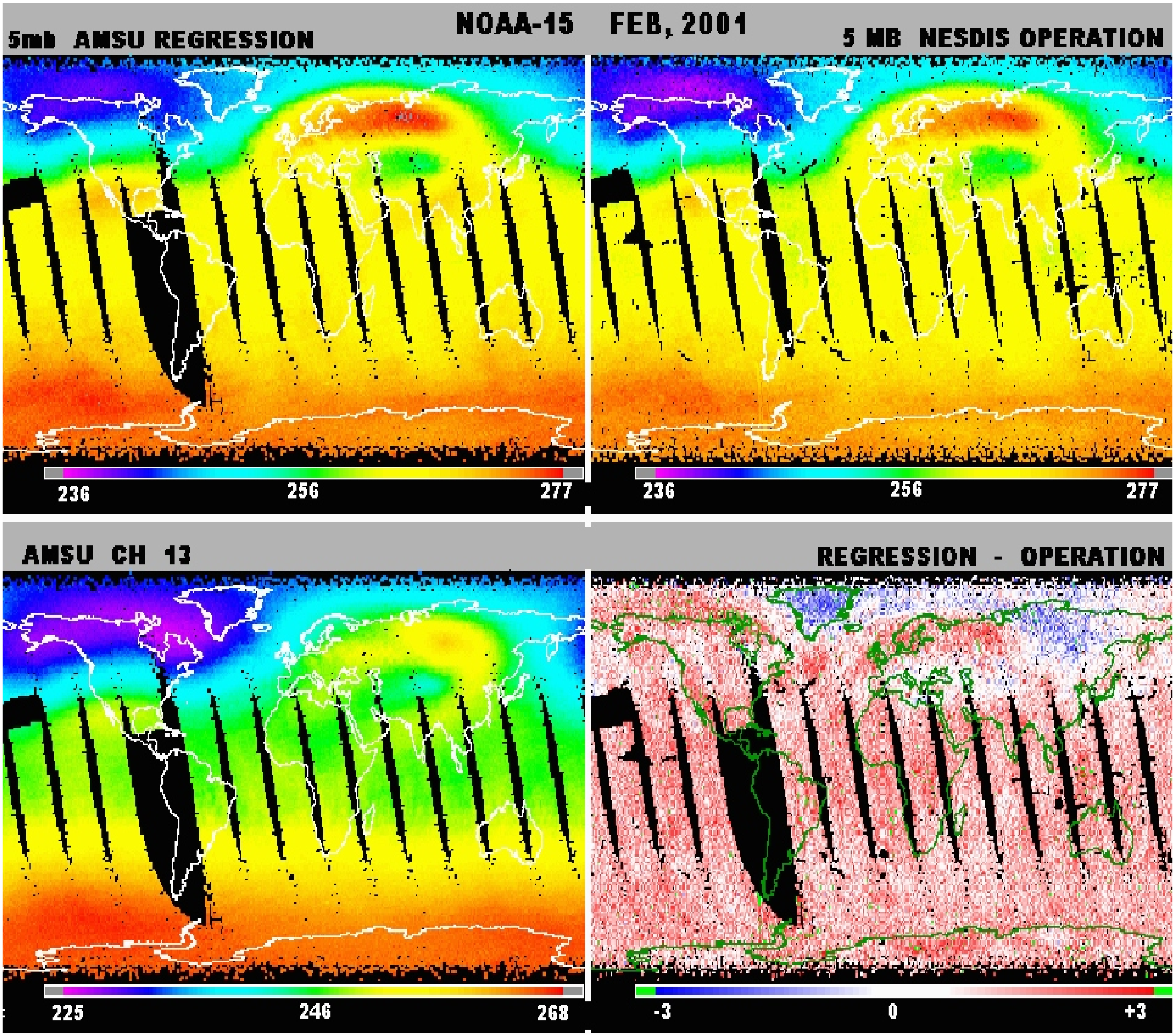

Figure 3: **Temperature at 5mb derived from AMSU-only Regression (upper left), the NESDIS Operation (upper right), the corresponding AMSU channel 13 radiance temperature measurements sensitive at the 5 mb level (lower left), and the Regression minus Operation differences at 5 mb (lower right), during February, 2001.**

A second question is why are there any differences at all. The answer is complex, but in summary these differences can be interpreted as a measure of the inherent uncertainty in any method which provides temperature estimates at these levels. This is attributable, for example, to uncertainties in radiative transfer physics, sounder measurements at these levels, and the sampling characteristics of the data used to generate coefficients. Assuming no changes, such differences can be expected to remain constant over time, with both solutions being equally creditable (equivalent).

The third question is why didn't NESDIS simply install the regression solution into orbital processing to compute upper stratospheric soundings. The primary reason was that the modification of offline systems is significantly less complex (from a system standpoint) than changes to online (orbital) systems. It was also understood that given the current first guess and retrieval approach operated by NESDIS, the proposed design was expected to yield similar results to installing it orbitally, while not introducing a bi-modal retrieval algorithm for the upper stratosphere versus the remaining atmosphere.

That the proposed design was expected to yield similar results from a direct installation into the orbital processing is based on the underlying NESDIS science which articulates that any reasonable estimate of first guess temperature and corresponding radiance temperature profiles is sufficient to retrieve sounding products which will satisfy the sounder observations (Fleming et al. 1986). Since the first guess temperatures in the upper stratosphere would now be based on the Goldberg regression (i.e., as appended above the highest radiosonde level), the final NESDIS retrieval and regression solutions were expected to converge in the upper stratosphere on a global scale. This is verified in Figures 2 and 3.

5 FUTURE PLANS

NESDIS' plans for ATOVS operational sounding systems include the replacement of the library search approach with an AMSU-only regression approach to compute the entire first guess profile. Users would then have the option to use the first guess profiles, for example, for climate applications, or the retrieved soundings, for real-time weather. Subsequent comparisons of the first guess and final temperature products in the upper stratosphere would likely exhibit differences consistent with those in Figure 3.

The availability of future systems to do this are currently planned early in 2002.

6 REFERENCES

Finger, F.G., M.E. Gelman, J.D. Wild, M.L. Chanin, A. Hauchecorne, and A.J. Miller, 1993: Evaluation of NMC upper-stratospheric temperature analysis using rocketsonde and lidar data. Bulletin of the American Meteorological Society, Vol 74, No. 5, 789-799.

Fleming, H.E., D.S. Crosby, and A.C. Neuendorffer, 1986: Correction of satellite temperature retrieval errors due to errors in atmospheric transmittances. Journal of Climate and Applied Meteorology, Vol 25, No. 6.

Goldberg, M.D., 1999: Generation of retrieval products from AMSU-A: methodology and validation Technical Proceedings of the 10th International TOVS Study Conference, Jan 26- Feb 2, Boulder, Colorado, USA.

Goldberg , M, J. Daniels and H. Fleming, 1988: A method for obtaining an improved initial approximation for the temperature/moisture retrieval problem. Preprints, 3rd Conference on satellite Meteorology and Oceanography, Anaheim, Ca, 16-19.

McMillin, L.M., L. Crone and T.J. Kleespies, 1995: Atmospheric transmittances of an absorbing gas. .Improvements to the OPTRAN approach. Appl. Opt., 34, 8396-8399

Reale, A.L., M.W. Chalfant, and L.M. Wilson, 2000: NESDIS advanced TOVS sounding products. 10th Conference on Satellite Meteorology and Oceanography, 9-14 January, Long Beach, Ca.

Tilley, F.H., M.E. Pettey, M.P. Ferguson, and A.L. Reale, 2000: Use of radiosondes in NESDIS advanced-TOVS (ATOVS) sounding products. 10th Conference on Satellite Meteorology and Oceanography, 9-14 January, Long Beach, Ca.

Wark, D.W., 1993: Adjustment of TIROS operational vertical sounder data to a vertical view. NOAA Technical Report NESDIS-64, U.S. Dept. Of Comm., Washington D.C., 36 pp.